10/ 618,414

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TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

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NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	DEC 05	CASREACT(R) - Over 10 million reactions available
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NEWS 5	DEC 14	2006 MeSH terms loaded for MEDLINE file segment of TOXCENTER
NEWS 6	DEC 14	CA/CAplus to be enhanced with updated IPC codes
NEWS 7	DEC 21	IPC search and display fields enhanced in CA/CAplus with the IPC reform
NEWS 8	DEC 23	New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/ USPAT2
NEWS 9	JAN 13	IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS 10	JAN 13	New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to INPADOC
NEWS 11	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS 12	JAN 17	IPC 8 in the WPI family of databases including WPIFV
NEWS 13	JAN 30	Saved answer limit increased
NEWS 14	JAN 31	Monthly current-awareness alert (SDI) frequency added to TULSA

NEWS EXPRESS JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT http://download.cas.org/express/v8.0-Discover/

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
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* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:00:14 ON 07 FEB 2006

=> file reg

10/ 618,414

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:00:56 ON 07 FEB 2006
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 6 FEB 2006 HIGHEST RN 873652-66-5
DICTIONARY FILE UPDATES: 6 FEB 2006 HIGHEST RN 873652-66-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

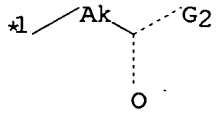
****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*
****

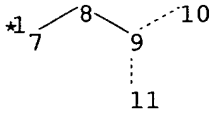
Structure search iteration limits have been increased. See HELP SLIMITS for details.

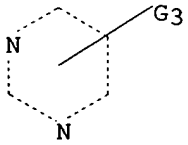
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

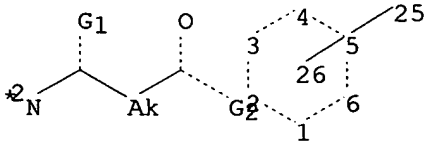
http://www.cas.org/ONLINE/UG/regprops.html

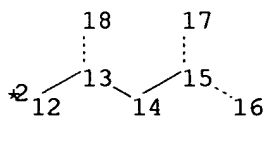
=>
Uploading C:\Program Files\Stnexp\Queries\10618414.str











chain nodes :
7 8 9 10 11 12 13 14 15 16 17 18 25
ring nodes :
1 2 3 4 5 6
chain bonds :
7-8 8-9 9-10 9-11 12-13 13-14 13-18 14-15 15-16 15-17

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 8-9 9-10 9-11 12-13 13-14 13-18 14-15
15-16 15-17
isolated ring systems :
containing 1 :

G1:H,O

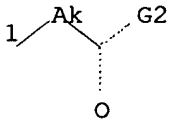
G2:O,N

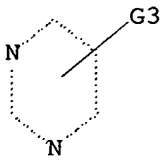
G3:[*1],[*2]

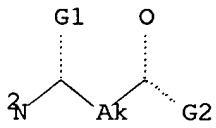
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
25:CLASS 26:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR







G1 H,O

G2 O,N

G3 [@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sample
SAMPLE SEARCH INITIATED 15:01:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 80165 TO ITERATE

2.5% PROCESSED 2000 ITERATIONS 9 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 1586473 TO 1620127

10/ 618,414

PROJECTED ANSWERS: 6075 TO 8353

L2 9 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 15:01:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1607858 TO ITERATE

60.7% PROCESSED 975397 ITERATIONS 2650 ANSWERS

62.2% PROCESSED 1000000 ITERATIONS 2663 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.18

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 1607858 TO 1607858
PROJECTED ANSWERS: 4085 TO 4477

L3 2663 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 167.38 167.59

FILE 'CAPLUS' ENTERED AT 15:02:16 ON 07 FEB 2006
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FILE COVERS 1907 - 7 Feb 2006 VOL 144 ISS 7
FILE LAST UPDATED: 6 Feb 2006 (20060206/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3
L4 365 L3

=> s l4 and (nanoic or nanoate)
1 NANOIC
11 NANOATE
L5 0 L4 AND (NANOIC OR NANOATE)

=> s l4 and acid
4097027 ACID
L6 249 L4 AND ACID

10/ 618,414

```
=> s l4 and (nonanoic or nonanoate)
          4584 NONANOIC
          1650 NONANOATE
L7           9 L4 AND (NONANOIC OR NONANOATE)

=> d his

     (FILE 'HOME' ENTERED AT 15:00:14 ON 07 FEB 2006)

     FILE 'REGISTRY' ENTERED AT 15:00:56 ON 07 FEB 2006
L1             STRUCTURE UPLOADED
L2           9 S L1 SAMPLE
L3        2663 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 15:02:16 ON 07 FEB 2006
L4         365 S L3
L5           0 S L4 AND (NANOIC OR NANOATE)
L6         249 S L4 AND ACID
L7           9 S L4 AND (NONANOIC OR NONANOATE)

=> d l7 1- ibib abs hitstr
YOU HAVE REQUESTED DATA FROM 9 ANSWERS - CONTINUE? Y/(N):y
```

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:756600 CAPLUS
DOCUMENT NUMBER: 141:277609
TITLE: Process for synthesizing intermediates, particularly fused pyridine derivatives, useful for the preparation of αvβ3 receptor antagonists such as (3S)-3-(2-methoxypyrimidin-5-yl)-5-oxo-9-(6,7,8,9-tetrahydro-5H-pyrido[2,3-b]azepin-2-yl) nonanoic acid and analogs
INVENTOR(S): Bishop, Brian Christopher; Brands, Karel Marie Joseph; Cottrell, Ian Frank; Cowden, Cameron John; Davies, Antony John; Keen, Stephen Philip; Lieberman, David Ross; Stewart, Gavin William
PATENT ASSIGNEE(S): Merck Sharp & Dohme Limited, UK; Merck & Co. Inc.
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004078109	A2	20040916	WO 2004-GB927	20040304
WO 2004078109	A3	20041118		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1603906	A2	20051214	EP 2004-717149	20040304
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				

PRIORITY APPLN. INFO.:
GB 2003-5277 A 20030307
GB 2003-5278 A 20030307
GB 2003-5284 A 20030307
WO 2004-GB927 W 20040304

OTHER SOURCE(S): CASREACT 141:277609; MARPAT 141:277609
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

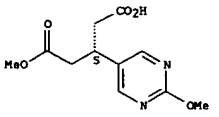
AB The invention relates to the synthesis of various intermediates useful in a multi-step preparation of compds. of formula I, wherein n is 2 or 3, and various salt forms of these compds. I are known compds., useful as αvβ3 receptor antagonists (no data). Thus, 1,1-dimethylethyl (6-chloro-2-pyridinyl)carbamate (II) was lithiated using hexyllithium and TMEDA in THF at -65° to -75°, and the resultant dianion was treated with Cl(CH2)4I, warmed, refluxed and worked up to give the cyclized intermediate III in 78% yield on a 5-kg scale. This chloride underwent Suzuki coupling with acrolein di-Et acetal via its

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
9-BBN adduct to give the corresponding 3-oxopropyl deriv., which underwent Wittig reaction with the corresponding triphenylphosphoranylidene ylide to give intermediate IV. This compd. underwent hydrogenation of the olefin, alk. sapon. of the ester, and removal of Boc with TFA, to give I (n = 3). This product was conveniently prepd. as a zwitterion, which has pharmaceutically advantageous soly. properties, by isolation from org. solvents such as CH2Cl2. A slurry of the zwitterion was converted to the TRIS salt by recrystn. from aq. iso-PrOH, and was obtained in 95% yield, 100% purity, and on a 4.40-kg scale for that final step. In the key chirality-generating step, the anhydride V (prepn. given) undergoes asym. solvolysis by MeOH in the presence of quinidine at -35° to -40°, giving the pure cryst. (S)-monoester VI in 63% yield and 98% enantiomeric excess (ee) without recrystn. Claims cover the exemplified process and variants thereof, for both the cases n = 2 and n = 3. The cyclization step was studied in detail for n = 1, 2, and 3. X-ray powder diffraction spectra are given for 2 polymorphs of VI, for I (n = 3), and for the TRIS salt of the latter.

IT **758686-06-5P**, (3S)-4-(Methoxycarbonyl)-3-(2-methoxypyrimidin-5-yl)butanoic acid
RL: IMF (Industrial manufacture); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; enantioselective process and intermediates for manufacture of (methoxypyrimidinyl)oxo(tetrahydropyridoazepinyl)nonanoic acid and analogs, useful as αvβ3 receptor antagonists)

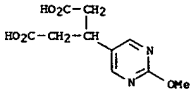
RN 758686-06-5 CAPLUS
CN Pentanedioic acid, 3-(2-methoxy-5-pyrimidinyl)-, monomethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



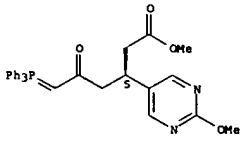
IT **758686-04-3P**, 4-Carboxy-3-(2-methoxypyrimidin-5-yl)butanoic acid
758686-07-6P, Methyl (3S)-3-(2-methoxypyrimidin-5-yl)-5-oxo-6-(triphenylphosphoranylidene)hexanoate **758686-08-7P**, tert-Butyl 2-[(7S)-8-methoxycarbonyl-7-(2-methoxypyrimidin-5-yl)-5-oxo-3-octenyl]-5,6,7,8-tetrahydropyrido[2,3-b]azepine-9-carboxylate **758686-09-8P**, tert-Butyl 2-[(7S)-8-methoxycarbonyl-7-(2-methoxypyrimidin-5-yl)-5-oxooctyl]-5,6,7,8-tetrahydropyrido[2,3-b]azepine-9-carboxylate **758686-10-1P**, tert-Butyl 2-[(7S)-8-carboxy-7-(2-methoxypyrimidin-5-yl)-5-oxooctyl]-5,6,7,8-tetrahydropyrido[2,3-b]azepine-9-carboxylate
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; enantioselective process and intermediates for manufacture of (methoxypyrimidinyl)oxo(tetrahydropyridoazepinyl)nonanoic acid and analogs, useful as αvβ3 receptor antagonists)

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 758686-04-3 CAPLUS
CN Pentanedioic acid, 3-(2-methoxy-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



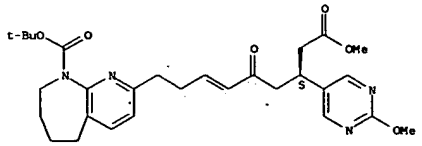
RN 758686-07-6 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methoxy-β-[2-oxo-3-(triphenylphosphoranylidene)propyl]-, methyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 758686-08-7 CAPLUS
CN 9H-Pyrido[2,3-b]azepine-9-carboxylic acid, 5,6,7,8-tetrahydro-2-[(7S)-9-methoxy-7-(2-methoxy-5-pyrimidinyl)-5,9-dioxo-3-nonenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

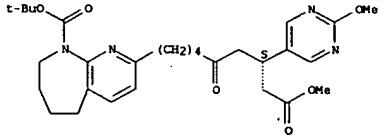
Absolute stereochemistry.
Double bond geometry unknown.



RN 758686-09-8 CAPLUS
CN 5H-Pyrido[2,3-b]azepine-2-nonanoic acid, 9-[(1,1-dimethylethoxy)carbonyl]-6,7,8,9-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, methyl ester, (βS)- (9CI) (CA INDEX NAME)

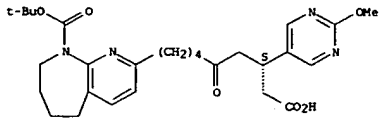
Absolute stereochemistry.

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 758686-10-1 CAPLUS
CN 5H-Pyrido[2,3-b]azepine-2-nonanoic acid, 9-[(1,1-dimethylethoxy)carbonyl]-6,7,8,9-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

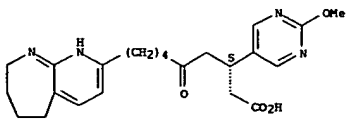
Absolute stereochemistry. Rotation (-).



IT **312262-25-2P**, (3S)-3-(2-Methoxypyrimidin-5-yl)-5-oxo-9-(6,7,8,9-tetrahydro-5H-pyrido[2,3-b]azepin-2-yl)nonanoic acid
RL: IMF (Industrial manufacture); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(target drug; enantioselective process and intermediates for manufacture of (methoxypyrimidinyl)oxo(tetrahydropyridoazepinyl)nonanoic acid and analogs, useful as αvβ3 receptor antagonists)

RN 312262-25-2 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



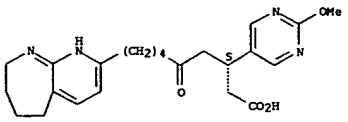
IT **758686-11-2P**, (3S)-3-(2-Methoxypyrimidin-5-yl)-5-oxo-9-(6,7,8,9-tetrahydro-5H-pyrido[2,3-b]azepin-2-yl)nonanoic acid TRIS salt
RL: IMF (Industrial manufacture); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(target drug; enantioselective process and intermediates for manufacture of

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(methoxypyrimidinyl)oxo(tetrahydropyridoazepinyl)nonanoic acid and analogs, useful as αvβ3 receptor antagonists)
RN 758686-11-2 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βS)-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

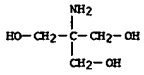
CRN 312262-25-2
CMF C23 H30 N4 O4

Absolute stereochemistry. Rotation (-).



CM 2

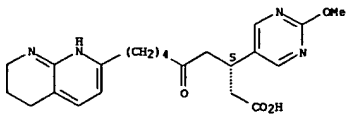
CRN 77-86-1
CMF C4 H11 N O3



IT **312262-16-1P**, (3S)-3-(2-Methoxypyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)nonanoic acid
758686-12-3P, (3S)-3-(2-Methoxypyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)nonanoic acid TRIS salt
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(target drug; enantioselective process and intermediates for manufacture of
(methoxypyrimidinyl)oxo(tetrahydropyridoazepinyl)nonanoic acid and analogs, useful as αvβ3 receptor antagonists)
RN 312262-16-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

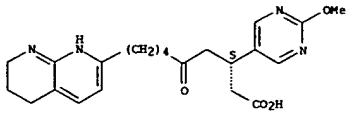


RN 758686-12-3 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βS)-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

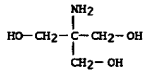
CRN 312262-16-1
CMF C22 H28 N4 O4

Absolute stereochemistry.



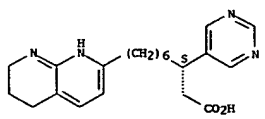
CM 2

CRN 77-86-1
CMF C4 H11 N O3



L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:694278 CAPLUS
DOCUMENT NUMBER: 141:325163
TITLE: Nonpeptide αvβ3 Antagonists. Part 11: Discovery and Preclinical Evaluation of Potent αvβ3 Antagonists for the Prevention and Treatment of Osteoporosis
AUTHOR(S): Coleman, Paul J.; Brashear, Karen M.; Askew, Ben C.; Hutchinson, John H.; McVean, Carol A.; Duong, Le T.; Feuston, Bradley P.; Fernandez-Metzler, Carmen; Gentile, Michael A.; Hartman, George D.; Kimmel, Donald B.; Leu, Chih-Tai; Lipfert, Lorraine; Merkle, Kara; Pennypacker, Brenda; Prueksaritanont, Thomayant; Rodan, Gideon A.; Wesolowski, Gregg A.; Rodan, Sevgi B.; Duggan, Mark E.
CORPORATE SOURCE: Departments of Medicinal Chemistry, Bone Biology and Osteporosis Research, Drug Metabolism and Pharmacology and Molecular Systems, Merck Research Laboratories, West Point, PA, 19486, USA
SOURCE: Journal of Medicinal Chemistry (2004), 47(20), 4829-4837
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:325163
AB 3-(S)-Pyrimidin-5-yl-9-(5,6,7,8-tetrahydro-[1,8]naphthyridin-2-yl)-nonanoic acid (5e) and 3-(S)-(methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-[1,8]naphthyridin-2-yl)-nonanoic acid (5f) were identified as potent and selective antagonists of the αvβ3 receptor. These compds. have excellent in vitro profiles (IC50 = 0.07 and 0.08 nM, resp.), significant unbound fractions in human plasma (6 and 4%), and good pharmacokinetics in rat, dog, and rhesus monkey. On the basis of the efficacy shown in an in vivo model of bone turnover following once-daily oral administration, these two compds. were selected for clin. development for the treatment of osteoporosis.
IT **227752-24-1P 227753-49-3P 227753-52-8P**
769936-46-1P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(nonpeptide αvβ3 antagonists in discovery and preclin. evaluation of potent αvβ3 antagonists for prevention and treatment of osteoporosis)
RN 227752-24-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-5-pyrimidinyl-, (βS)- (9CI) (CA INDEX NAME)

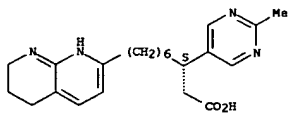
Absolute stereochemistry.



RN 227753-49-3 CAPLUS

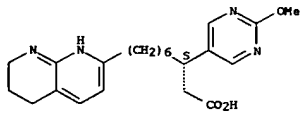
L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



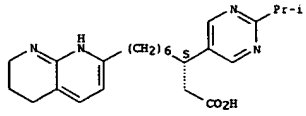
RN 227753-52-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 769936-46-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-[2-(1-methylethyl)-5-pyrimidinyl]-, (βS)- (9CI) (CA INDEX NAME)

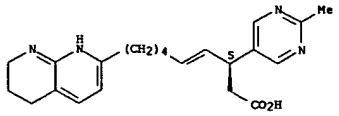
Absolute stereochemistry.



IT **769936-69-8P 769936-70-1P 769936-71-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(nonpeptide αvβ3 antagonists in discovery and preclin. evaluation of potent αvβ3 antagonists for prevention and treatment of osteoporosis)
RN 769936-69-8 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methyl-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, (βS)- (9CI) (CA INDEX NAME)

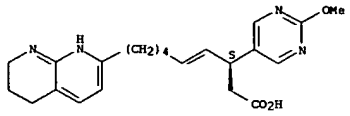
Absolute stereochemistry.
Double bond geometry unknown.

L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



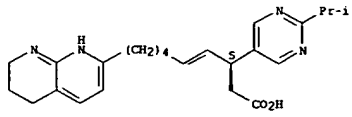
RN 769936-70-1 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methoxy-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



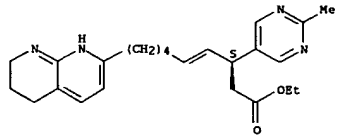
RN 769936-71-2 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-(1-methylethyl)-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



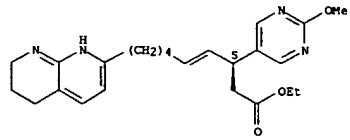
IT **227752-22-9P 769936-34-7P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(nonpeptide αvβ3 antagonists in discovery and preclin. evaluation of potent αvβ3 antagonists for prevention and treatment of osteoporosis)
RN 227752-22-9 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-5-pyrimidinyl-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



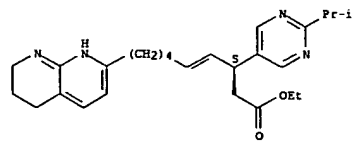
RN 769936-64-3 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methoxy-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



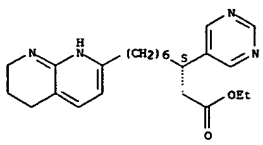
RN 769936-65-4 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-(1-methylethyl)-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, ethyl ester, (βS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



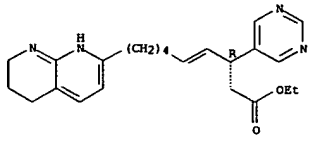
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.



RN 769936-34-7 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, ethyl ester, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



IT **431040-43-6P 769936-64-3P 769936-65-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(nonpeptide αvβ3 antagonists in discovery and preclin. evaluation of potent αvβ3 antagonists for prevention and treatment of osteoporosis)
RN 431040-43-6 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methyl-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

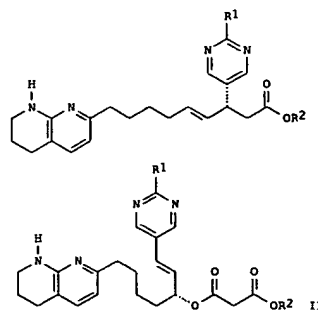
L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:696685 CAPLUS
DOCUMENT NUMBER: 139:230784
TITLE: Malonate-Claisen rearrangement for preparation of integrin receptor antagonist intermediates
INVENTOR(S): Humphrey, Guy R.; Farr, Roger N.; Lee, Jaemoon
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003072042	A2	20030904	WO 2003-US5476	20030221
WO 2003072042	A3	20040304		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2002-360273P P 20020227
OTHER SOURCE(S): CASREACT 139:230784; MARPAT 139:230784
GI



I

II

AB A process is described for the preparation of chiral unsatd. ester

L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

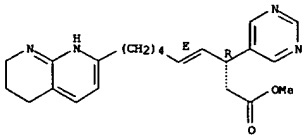
intermediates [I; having the (R)-configuration at the stereogenic center marked with *; R1 = H, methyl; R2 = C1-4 alkyl, phenyl-C1-3-alkyl; e.g., 3-(R)-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)-(E)-non-4-enoic acid Me ester], useful in the asym. syntheses of αvβ3 integrin receptor antagonists (no data), which involves an efficient Claisen rearrangement of a malonate ester of a chiral allylic alc. precursor [II; e.g., Et malonate ester of (R)-1-(pyrimidin-5-yl)-7-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)-(E)-hept-1-en-3-ol] followed by hydrolysis and decarboxylation. The unsatd. ester intermediates can be converted in a 2-step sequence into the desired substituted nonanoic acid derivs. [e.g., 3-(S)-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid Me ester].

IT **593282-80-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in a malonate-Claisen rearrangement for preparation of integrin receptor antagonist intermediates)

RN 593282-80-5 CAPLUS

CN 5-Pyrimidinepropanoic acid, β-[(1E)-6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, methyl ester, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



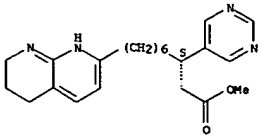
IT **593282-81-6P 593282-82-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(malonate-Claisen rearrangement for preparation of integrin receptor antagonist intermediates)

RN 593282-81-6 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-5-pyrimidinyl-, methyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

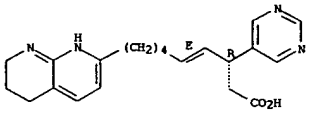
L7 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 593282-82-7 CAPLUS

CN 5-Pyrimidinepropanoic acid, β-[(1E)-6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

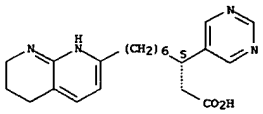


IT **227752-24-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(malonate-Claisen rearrangement for preparation of integrin receptor antagonist intermediates)

RN 227752-24-1 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-5-pyrimidinyl-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:977654 CAPLUS
DOCUMENT NUMBER: 138:61306
TITLE: Preparation of pharmaceuticals containing (pyrimidinyl)tetrahydronaphthyridinylnonanoic acid Tris salt as an integrin receptor antagonist
INVENTOR(S): Humphrey, Guy R.; Xu, Wei
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 21 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002102374	A1	20021227	WO 2002-US18906	20020614
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003004171	A1	20030102	US 2002-174016	20020618
US 6750220	B2	20040615		

PRIORITY APPLN. INFO.: US 2001-299344P P 20010619

AB The tris(hydroxymethyl)aminomethane ("TRIS") salt of 3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-[1,8]-naphthyridin-2-yl)nonanoic acid is a potent antagonist of the integrin αvβ3 receptor and is useful for the prevention and/or treatment of osteoporosis and vascular restenosis, as well as conditions associated with excessive angiogenesis, such as macular degeneration, diabetic retinopathy, atherosclerosis, inflammatory arthritis, cancer, and metastatic tumor growth. The invention also relates to a process for the preparation of the salt as well as pharmaceutical compns. containing the salt and methods of using the salt. Thus, the 3R or 3S isomer of 3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-[1,8]-naphthyridin-2-yl)nonanoic acid was treated with tris(hydroxymethyl)aminomethane in EtOH solution to give the title salts. The products were characterized by x-ray diffraction and FT-IR spectra and DSC. A 100-mg tablet is composed of 133 mg the active ingredient, 243 mg lactose, 20 mg croscarmellose sodium, and 4 mg magnesium stearate.

IT **479063-88-2P 479063-90-6P 479063-93-9P**
RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pharmaceuticals containing (pyrimidinyl)tetrahydronaphthyridinyl nonanoic acid Tris salt as integrin receptor antagonist)

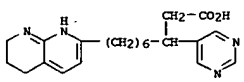
RN 479063-88-2 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-5-pyrimidinyl-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

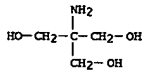
CRN 227753-43-7
CMF C21 H28 N4 O2

L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

CRN 77-86-1
CMF C4 H11 N O3



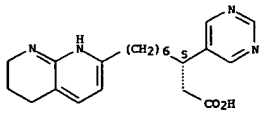
RN 479063-90-6 CAPLUS

CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-5-pyrimidinyl-, (βS)-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

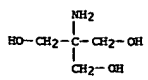
CRN 227752-24-1
CMF C21 H28 N4 O2

Absolute stereochemistry.



CM 2

CRN 77-86-1
CMF C4 H11 N O3



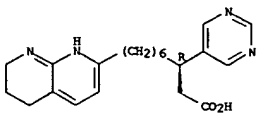
RN 479063-93-9 CAPLUS

L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-5-pyrimidinyl-, (βR)-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

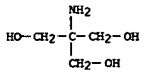
CRN 227752-23-0
CMF C21 H28 N4 O2

Absolute stereochemistry.



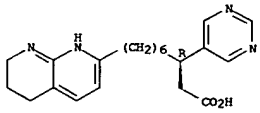
CM 2

CRN 77-86-1
CMF C4 H11 N O3



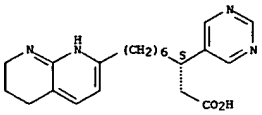
IT 227752-23-0 227752-24-1 227753-43-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pharmaceuticals containing (pyrimidinyl)tetrahydronaphthyridinyl nonanoic acid Tris salt as integrin receptor antagonist)
RN 227752-23-0 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-5-pyrimidinyl-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

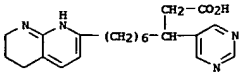


L7 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 227752-24-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-5-pyrimidinyl-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 227753-43-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-5-pyrimidinyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:409266 CAPLUS
DOCUMENT NUMBER: 136:409377
TITLE: Preparation of amine salts of an integrin receptor antagonist
INVENTOR(S): Humphrey, Guy R.; Waters, Marjorie See; Xu, Wei
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 21 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002065291	A1	20020530	US 2001-998416	20011129
US 6444680	B2	20020903		

PRIORITY APPLN. INFO.: US 2000-250268P P 20001130

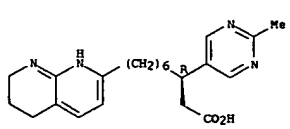
AB Amine salts of 3-(2-methyl-pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-[1,8]-naphthyridin-2-yl)nonanoic acid are potent antagonists of the integrin αvβ3 receptor and are useful for the prevention and/or treatment of osteoporosis and vascular restenosis, as well as conditions associated with excessive angiogenesis, such as macular degeneration, diabetic retinopathy, atherosclerosis, inflammatory arthritis, cancer, and metastatic tumor growth. The invention also relates to a process for the preparation of the novel salts as well as pharmaceutical compns. containing the salts and methods of using the salts. Also disclosed are 3(R)- and 3(S)-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-[1,8]naphthyridin-2-yl)nonanoic acid (I) in the form of a zwitterion trihydrate. Thus, I were prepared in a series of steps. A 100-mg tablet was composed of 100 mg active ingredient, 276 mg mannitol, 20 mg of croscarmellose sodium, and 4 mg magnesium stearate.

IT 431040-45-8P 431040-46-9P 431040-47-0P 431040-48-1P 431040-49-2P 431040-50-5P
RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amine salts of integrin receptor antagonist)
RN 431040-45-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βR)-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 227753-48-2
CMF C22 H30 N4 O2

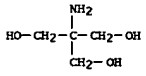
Absolute stereochemistry.



L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 77-86-1
CMF C4 H11 N O3

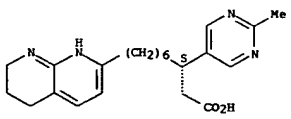


RN 431040-46-9 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βS)-, compd. with 2-amino-2-(hydroxymethyl)-1,3-propanediol (1:1) (9CI) (CA INDEX NAME)

CM 1

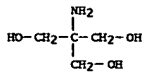
CRN 227753-49-3
CMF C22 H30 N4 O2

Absolute stereochemistry.



CM 2

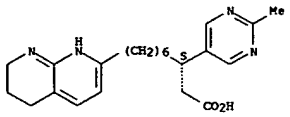
CRN 77-86-1
CMF C4 H11 N O3



RN 431040-47-0 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, trihydrate, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

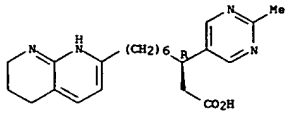
L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



●3 H_2O

RN 431040-48-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, trihydrate, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



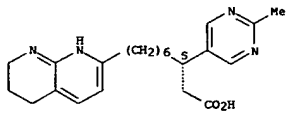
●3 H_2O

RN 431040-49-2 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βS)-, compd. with 2-amino-2-methyl-1-propanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 227753-49-3
CMF C22 H30 N4 O2

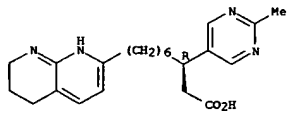
Absolute stereochemistry.



L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

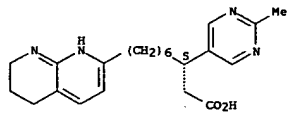
RN 227753-48-2 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



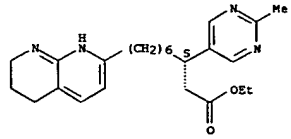
RN 227753-49-3 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 404869-67-6 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



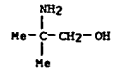
RN 431040-42-5 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methyl-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, ethyl ester, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 124-68-5
CMF C4 H11 N O

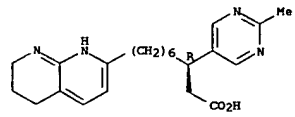


RN 431040-50-5 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βR)-, compd. with 2-amino-2-methyl-1-propanol (1:1) (9CI) (CA INDEX NAME)

CM 1

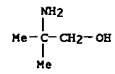
CRN 227753-48-2
CMF C22 H30 N4 O2

Absolute stereochemistry.



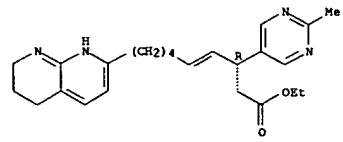
CM 2

CRN 124-68-5
CMF C4 H11 N O



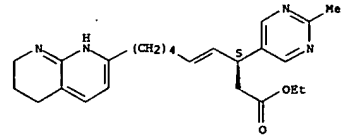
IT **227753-48-2P 227753-49-3P 404869-67-6P**
431040-42-5P 431040-43-6P 431040-44-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amine salts of integrin receptor antagonist)

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



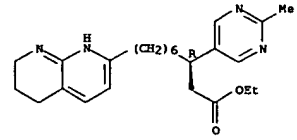
RN 431040-43-6 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methyl-β-[6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-hexenyl]-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



RN 431040-44-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, ethyl ester, (βR)- (9CI) (CA INDEX NAME)

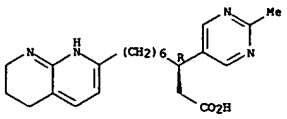
Absolute stereochemistry.



IT **431040-51-6P 431040-52-7P 431040-53-8P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amine salts of integrin receptor antagonist)
RN 431040-51-6 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, monoammonium salt, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



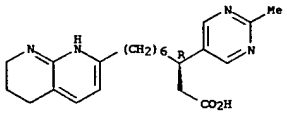
● NH_3

RN 431040-52-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βR)-, compd. with 1,2-ethanediamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 227753-48-2
CMF C22 H30 N4 O2

Absolute stereochemistry.



CM 2

CRN 107-15-3
CMF C2 H8 N2

$H_2N-CH_2-CH_2-NH_2$

RN 431040-53-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βR)-, compd. with N-(phenylmethyl)benzenemethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

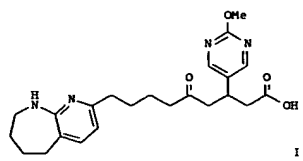
CRN 227753-48-2
CMF C22 H30 N4 O2

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:275794 CAPLUS
DOCUMENT NUMBER: 136:309803
TITLE: Preparation of a phosphoric acid salt of an integrin receptor antagonist
INVENTOR(S): Meissner, Robert S.; Xu, Wei
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 27 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002028395	A1	20020411	WO 2001-US30647	20011001
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2424117	AA	20020411	CA 2001-2424117	20011001
AU 2001096439	A5	20020415	AU 2001-96439	20011001
EP 1326615	A1	20030716	EP 2001-977309	20011001
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004510738	T2	20040408	JP 2002-532220	20011001
US 2005101593	A1	20050512	US 2003-398366	20011001
PRIORITY APPLN. INFO.:			US 2000-237534P P	20001004
			WO 2001-US30647 W	20011001

GI

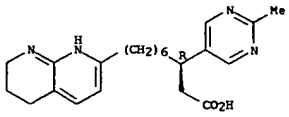


I

AB The phosphoric acid salt of 3-(2-methoxy-pyrimidin-5-yl)-5-oxo-9-(6,7,8,9-tetrahydro-5H-pyrido[2,3-b]azepin- -yl)-nonanoic acid (I) is a potent antagonist of the integrin αvβ3 receptor and is useful for the prevention and/or treatment of osteoporosis and vascular restenosis, as well as conditions associated with excessive angiogenesis, such as macular degeneration, diabetic retinopathy, atherosclerosis, inflammatory arthritis, cancer, and metastatic tumor growth. The

L7 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.



CM 2

CRN 103-49-1
CMF C14 H15 N

Ph-CH_2-NH-CH_2-Ph

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

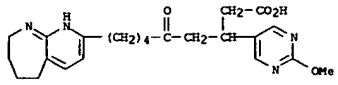
invention also relates to a process for the prepn. of the novel salt as well as pharmaceutical compns. and methods of use. Thus, I·H3PO4 was prepd. from I Et ester via sapon. with aq. NaOH followed by reaction of H3PO4 in EtOH. The the crystal structure of I·H3PO4 was detd. via x-ray powder diffraction.

IT 408357-11-9P 408357-12-0P 408357-13-1P
RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of crystalline phosphoric acid salt of integrin αvβ3 receptor antagonist useful as therapeutic for osteoporosis and vascular restenosis)

RN 408357-11-9 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, phosphate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 312262-23-0
CMF C23 H30 N4 O4



CM 2

CRN 7664-38-2
CMF H3 O4 P

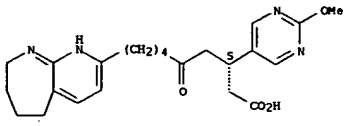
RN 408357-12-0 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βS)-, phosphate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 312262-25-2
CMF C23 H30 N4 O4

Absolute stereochemistry. Rotation (-).

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

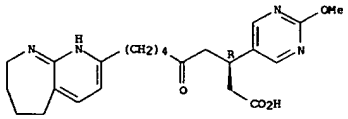
CRN 7664-38-2
CMF H3 O4 P

RN 408357-13-1 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βR)-, phosphate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 312262-24-1
CMF C23 H30 N4 O4

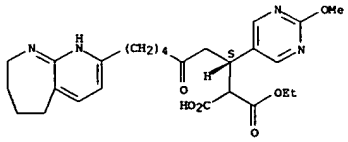
Absolute stereochemistry.



CM 2

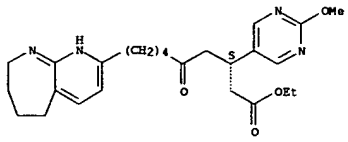
CRN 7664-38-2
CMF H3 O4 P

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.



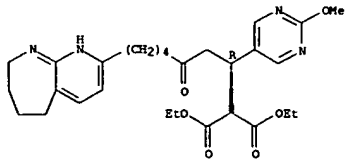
RN 408357-21-1 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 408357-23-3 CAPLUS
CN Propanedioic acid, [(1R)-1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(5,6,7,8-tetrahydro-1H-pyrido[2,3-b]azepin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

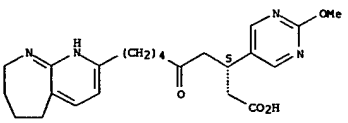


IT 312262-23-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of crystalline phosphoric acid salt of integrin αvβ3 receptor antagonist useful as therapeutic for osteoporosis and vascular restenosis)
RN 312262-23-0 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

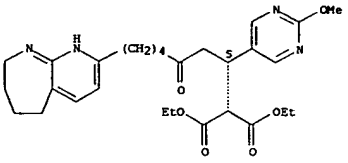
IT 312262-25-2P 408357-19-7P 408357-20-0P
408357-21-1P 408357-23-3P
RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of crystalline phosphoric acid salt of integrin αvβ3 receptor antagonist useful as therapeutic for osteoporosis and vascular restenosis)
RN 312262-25-2 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



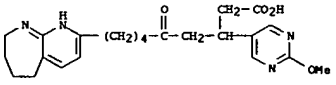
RN 408357-19-7 CAPLUS
CN Propanedioic acid, [(1S)-1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(5,6,7,8-tetrahydro-1H-pyrido[2,3-b]azepin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



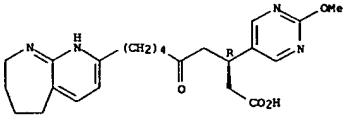
RN 408357-20-0 CAPLUS
CN Propanedioic acid, [(1S)-1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(5,6,7,8-tetrahydro-1H-pyrido[2,3-b]azepin-2-yl)heptyl]-, monoethyl ester (9CI) (CA INDEX NAME)

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
methoxy-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)

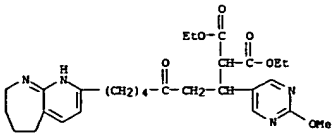


IT 312262-24-1P 408357-18-6P 408357-25-5P
408357-27-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of crystalline phosphoric acid salt of integrin αvβ3 receptor antagonist useful as therapeutic for osteoporosis and vascular restenosis)
RN 312262-24-1 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



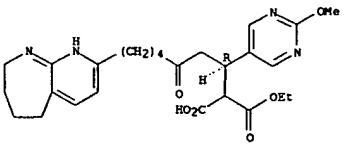
RN 408357-18-6 CAPLUS
CN Propanedioic acid, [1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(5,6,7,8-tetrahydro-1H-pyrido[2,3-b]azepin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 408357-25-5 CAPLUS
CN Propanedioic acid, [(1R)-1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(5,6,7,8-tetrahydro-1H-pyrido[2,3-b]azepin-2-yl)heptyl]-, monoethyl ester (9CI) (CA INDEX NAME)

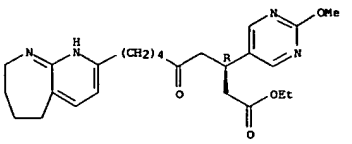
Absolute stereochemistry.

L7 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

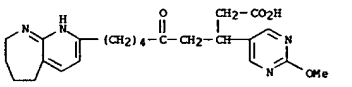


RN 408357-27-7 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-8-oxo-, ethyl ester, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 312262-23-0DP, salt
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of crystalline phosphoric acid salt of integrin αvβ3 receptor antagonist useful as therapeutic for osteoporosis and vascular restenosis)
RN 312262-23-0 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-8-oxo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:89834 CAPLUS
DOCUMENT NUMBER: 136:134745
TITLE: Preparation of heterocycle-substituted chain-fluorinated carboxylic acids and esters useful as αv integrin receptor antagonists
INVENTOR(S): Wang, Jiabing
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002007730	A1	20020131	WO 2001-US22938	20010720
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2416751	AA	20020131	CA 2001-2416751	20010720
AU 2001077935	A5	20020205	AU 2001-77935	20010720
EP 1315501	A1	20030604	EP 2001-955884	20010720
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004504349	T2	20040212	JP 2002-513465	20010720
US 2004038963	A1	20040226	US 2002-276048	20021112
PRIORITY APPLN. INFO.:			US 2000-220903P	P 20000726
			WO 2001-US22938	W 20010720

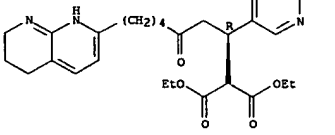
OTHER SOURCE(S): MARPAT 136:134745

AB The present invention relates to novel chain-fluorinated alkanoic acid derivs. XCH2CH2CR3(2CH2CR4(2CH2CHR5CH2CO2R6 (I; e.g. (3S)-5,5-difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl) nonanoic acid), their synthesis, and their use as αv integrin receptor antagonists. More particularly, the compds. of the present invention are antagonists of the integrin receptors αvβ3 and/or αvβ5 and are useful for inhibiting bone resorption, treating and preventing osteoporosis, and inhibiting vascular restenosis, diabetic retinopathy, macular degeneration, angiogenesis, atherosclerosis, inflammation, inflammatory arthritis, viral disease, cancer, and metastatic tumor growth. In I, X = 5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl, 2,3-dihydro-1H-pyrrolo[2,3-b]pyridin-2-yl, 5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl, or 6-R2NHpyridin-2-yl, wherein each nonarom. ring C atom is unsubstituted or independently substituted with one or two R1 substituents and each aromatic ring C atom is unsubstituted or independently substituted with one R1 substituent. R1 = C1-8 alkyl, C3-8 cycloalkyl, C3-8 cycloheteroalkyl, C3-8 cycloalkyl-C1-6 alkyl, C3-8 cycloheteroalkyl-C1-6 alkyl, aryl, aryl-C1-6 alkyl, amino, amino-C1-6 alkyl, C1-3 acylamino, C1-3 acylamino-C1-6 alkyl, (C1-6 alkyl)1-2-amino, C3-6 cycloalkyl-C0-2 amino, (C1-6 alkyl)1-2-amino-C1-6-

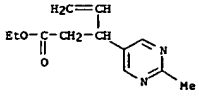
L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
alkyl, C1-6 alkoxy, C1-4 alkoxy-C1-6 alkyl, hydroxycarbonyl, hydroxycarbonyl-C1-6 alkyl, C1-3 alkoxycarbonyl, C1-3 alkoxycarbonyl-C1-6 alkyl, hydroxy, hydroxy-C1-6-alkyl, nitro, cyano, trifluoromethyl, trifluoromethoxy, trifluoroethoxy, C1-8 alkyl-S(O)0-2, (C1-8 alkyl)0-2-aminocarbonyl, C1-8 alkyloxycarbonylamino, (C1-8 alkyl)1-2-aminocarbonyloxy, (aryl C1-3 alkyl)1-2-amino, (aryl)1-2-amino, aryl-C1-3 alkylsulfonylamino, and C1-8 alkylsulfonylamino; or two R1 substituents, when on the same nonarom. C atom, are taken together with the C atom to which they are attached to form a carbonyl group, or two R1 substituents, together with the nonarom. C atoms to which they are attached, join to form a 4- to 6-membered satd. or unsatd. carbocyclic ring. R2 is H or C1-4 alkyl; R3 is fluoro and R4 is H or R3 is H and R4 is fluoro. Although the methods of prepn. are not claimed, approx.10 example prepns. are included. Representative compds. of the present invention were tested and found to bind to human αvβ3 integrin. These compds. were generally found to have IC50 values <10 nM in the SPAV3 assay. Representative compds. of the present invention were also tested in the SPAV5 assay to det. affinity for the αvβ5 receptor. These compds. were generally found to have IC50 values <100 nM.
IT 312262-91-2P, 2-[(1R)-(2-Methylpyrimidin-5-yl)-3-oxo-7-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)heptyl]malonic acid diethyl ester 312262-95-6P, 3-(2-Methylpyrimidin-5-yl)pent-4-enoic acid ethyl ester 312262-96-7P, 5-Hydroxy-3-(2-methylpyrimidin-5-yl)pentanoic acid ethyl ester 312262-97-8P, 3-(2-Methylpyrimidin-5-yl)-5-oxopentanoic acid ethyl ester 312263-52-8P, 2-[(1S)-(2-Methylpyrimidin-5-yl)-3-oxo-7-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)heptyl]malonic acid diethyl ester 393177-66-7P, (3S)-3-(2-Methylpyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-67-8P, (3S)-5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-69-0P, (3R)-3-(2-Methylpyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-71-4P, (3S)-3-(2-Methylpyrimidin-5-yl)-5-oxo-9-(3-cyclopropyl-5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-72-5P, (3R)-3-(2-Methylpyrimidin-5-yl)-5-oxo-9-(3-cyclopropyl-5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl) nonanoic acid ethyl ester 393177-73-6P, (3S)-9-(3-Cyclopropyl-5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)-5,5-difluoro-3-(2-methylpyrimidin-5-yl)nonanoic acid ethyl ester 393177-76-9P, (3S)-3-(2-Methoxypyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-77-0P, (3R)-3-(2-Methoxypyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-78-1P, (3S)-5,5-Difluoro-3-(2-methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-80-5P, (3S)-3-(2-Methoxypyrimidin-5-yl)-4-[2-[4-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)butyl]-1,3-dithioan-2-yl]butanoic acid ethyl ester 393177-81-6P, (3S)-5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(3-bromo-5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-82-7P, 3-(2-Methylpyrimidin-5-yl)-7-oxo-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)nonanoic acid ethyl ester 393177-86-1P, 3-(2-Methylpyrimidin-5-yl)-7-oxo-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)-non-5-enoic acid ethyl ester 393177-87-2P, (3S)-3-(2-Methylpyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)nonanoic acid ethyl ester 393177-88-3P, (3R)-3-(2-Methylpyrimidin-5-yl)-5-oxo-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)nonanoic acid ethyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(Reactant or reagent)
(intermediate; prepn. of heterocycle-substituted chain-fluorinated carboxylic acids and esters useful as αv integrin receptor antagonists)
RN 312262-91-2 CAPLUS
CN Propanedioic acid, [(1R)-1-(2-methyl-5-pyrimidinyl)-3-oxo-7-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

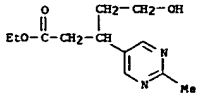
Absolute stereochemistry.



RN 312262-95-6 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-ethenyl-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)

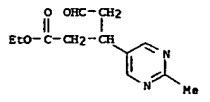


RN 312262-96-7 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-(2-hydroxyethyl)-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)



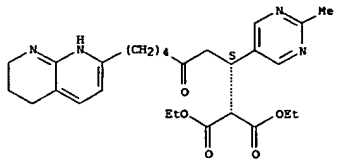
RN 312262-97-8 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methyl-β-(2-oxoethyl)-, ethyl ester (9CI) (CA INDEX NAME)

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



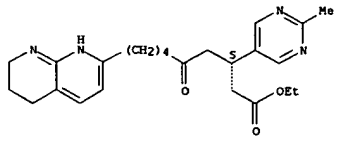
RN 312263-52-8 CAPLUS
CN Propanedioic acid, [(1S)-1-(2-methyl-5-pyrimidinyl)-3-oxo-7-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 393177-66-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

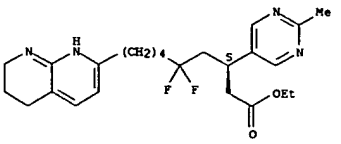
Absolute stereochemistry.



RN 393177-67-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

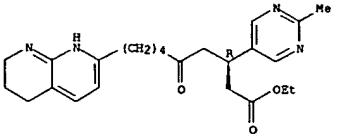
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



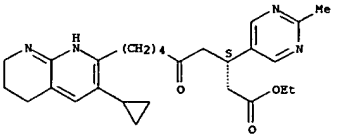
RN 393177-69-0 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, ethyl ester, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 393177-71-4 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

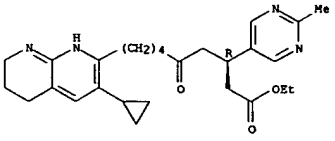
Absolute stereochemistry.



RN 393177-72-5 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, ethyl ester, (βR)- (9CI) (CA INDEX NAME)

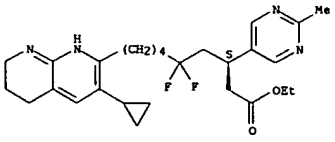
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



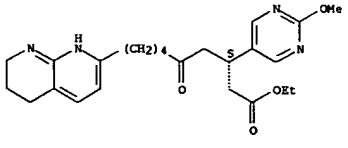
RN 393177-73-6 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 393177-76-9 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

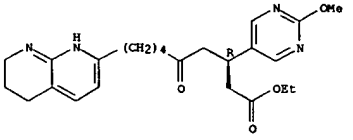
Absolute stereochemistry.



RN 393177-77-0 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, ethyl ester, (βR)- (9CI) (CA INDEX NAME)

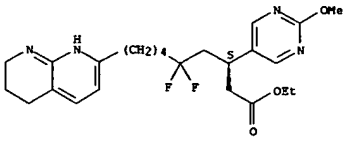
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



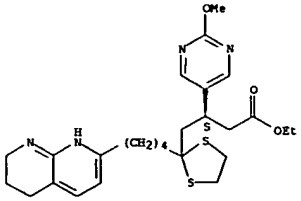
RN 393177-78-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



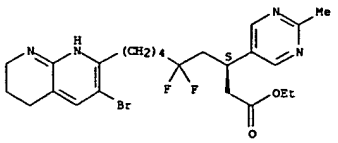
RN 393177-80-5 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methoxy-β-[[2-[4-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)butyl]-1,3-dithiolan-2-yl]methyl]-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

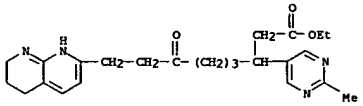


RN 393177-81-6 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-bromo-δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

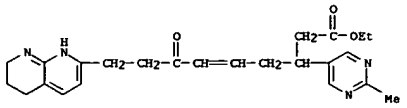
L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.



RN 393177-82-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-ζ-oxo-, ethyl ester (9CI) (CA INDEX NAME)



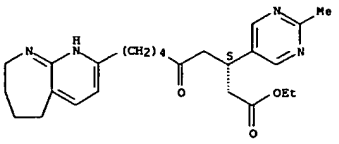
RN 393177-86-1 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methyl-β-[4-oxo-6-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-2-hexenyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 393177-87-2 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, ethyl ester, (βS)- (9CI) (CA INDEX NAME)

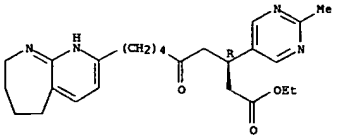
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 393177-88-3 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, ethyl ester, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

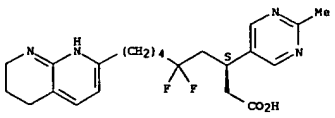


IT **393177-64-5P**, (3S)-5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)**nonanoic** acid **393177-68-9P**, (3R)-5,5-Difluoro-3-(2-Methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)**nonanoic** acid **393177-70-3P**, (3S)-9-(3-Cyclopropyl-5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)-5,5-difluoro-3-(2-methylpyrimidin-5-yl) **nonanoic** acid **393177-74-7P**, (3R)-9-(3-Cyclopropyl-5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)-5,5-difluoro-3-(2-methylpyrimidin-5-yl)**nonanoic** acid **393177-75-8P**, (3S)-5,5-Difluoro-3-(2-Methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)**nonanoic** acid **393177-79-2P**, (3R)-5,5-Difluoro-3-(2-Methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)**nonanoic** acid **393177-89-4P**, 5,5-Difluoro-3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)**nonanoic** acid **393177-90-7P**, (3S)-5,5-Difluoro-3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)**nonanoic** acid **393177-91-8P**, (3R)-5,5-Difluoro-3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)**nonanoic** acid **393177-92-9P**, 5,5-Difluoro-3-(2-methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)**nonanoic** acid **393177-93-0P**, 5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro[1,8]naphthyridin-2-yl)**nonanoic** acid **393177-94-1P**, 9-(3-Cyclopropyl-5,6,7,8-tetrahydro[1,8]naphthyridin-

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
2-yl)-5,5-difluoro-3-(2-methylpyrimidin-5-yl)**nonanoic** acid **393177-95-2P**, 5,5-Difluoro-3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)**nonanoic** acid **393177-96-3P**, (3S)-5,5-Difluoro-3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)**nonanoic** acid **393177-97-4P**, (3R)-5,5-Difluoro-3-(pyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)**nonanoic** acid **393177-98-5P**, 5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)**nonanoic** acid **393177-99-6P**, (3S)-5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)**nonanoic** acid **393178-00-2P**, (3R)-5,5-Difluoro-3-(2-methylpyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)**nonanoic** acid **393178-01-3P**, 5,5-Difluoro-3-(2-methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)**nonanoic** acid **393178-02-4P**, (3S)-5,5-Difluoro-3-(2-methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)**nonanoic** acid **393178-03-5P**, (3R)-5,5-Difluoro-3-(2-methoxypyrimidin-5-yl)-9-(5,6,7,8-tetrahydro-9H-pyrido[2,3-b]azepin-2-yl)**nonanoic** acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of heterocycle-substituted chain-fluorinated carboxylic acids and esters useful as αv integrin receptor antagonists)

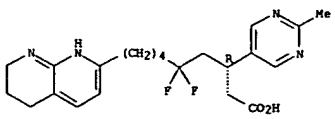
RN 393177-64-5 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 393177-68-9 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βR)- (9CI) (CA INDEX NAME)

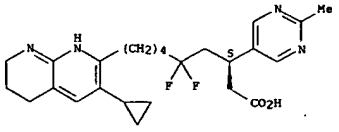
Absolute stereochemistry.



RN 393177-70-3 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-δ,δ-difluoro-

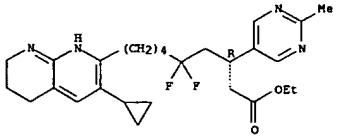
L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



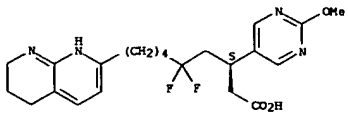
RN 393177-74-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, ethyl ester, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 393177-75-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-, (βS)- (9CI) (CA INDEX NAME)

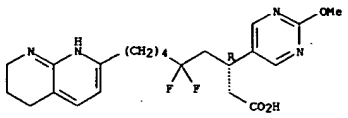
Absolute stereochemistry.



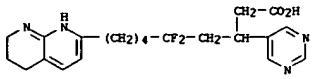
RN 393177-79-2 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

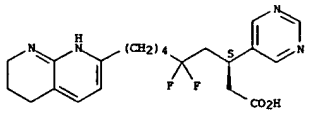


RN 393177-89-4 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-5-pyrimidinyl- (9CI) (CA INDEX NAME)



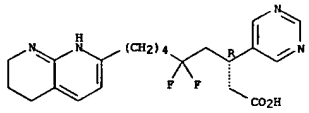
RN 393177-90-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-5-pyrimidinyl-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



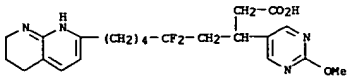
RN 393177-91-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-5-pyrimidinyl-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

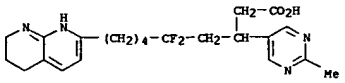


RN 393177-92-9 CAPLUS

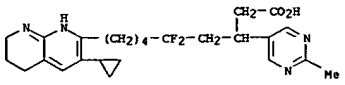
L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



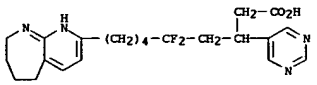
RN 393177-93-0 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



RN 393177-94-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-δ,δ-difluoro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



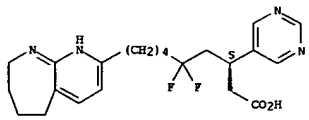
RN 393177-95-2 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, δ,δ-difluoro-5,6,7,8-tetrahydro-β-5-pyrimidinyl- (9CI) (CA INDEX NAME)



RN 393177-96-3 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, δ,δ-difluoro-5,6,7,8-tetrahydro-β-5-pyrimidinyl-, (βS)- (9CI) (CA INDEX NAME)

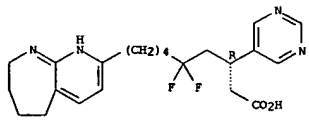
Absolute stereochemistry.

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

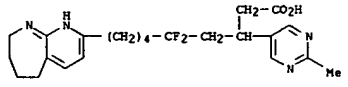


RN 393177-97-4 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, δ,δ-difluoro-5,6,7,8-tetrahydro-β-5-pyrimidinyl-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

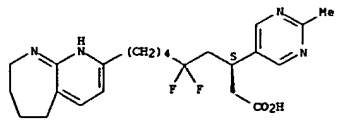


RN 393177-98-5 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, δ,δ-difluoro-5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



RN 393177-99-6 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, δ,δ-difluoro-5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βS)- (9CI) (CA INDEX NAME)

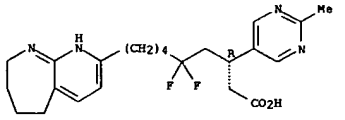
Absolute stereochemistry.



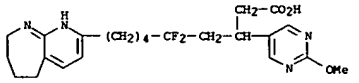
RN 393178-00-2 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, δ,δ-difluoro-5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-, (βR)- (9CI) (CA INDEX

L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
NAME)

Absolute stereochemistry.

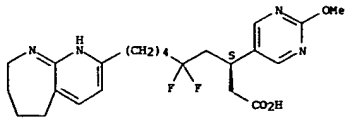


RN 393178-01-3 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, δ,δ-difluoro-5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



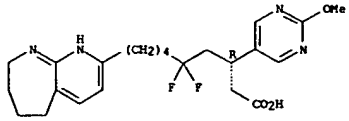
RN 393178-02-4 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, δ,δ-difluoro-5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 393178-03-5 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, δ,δ-difluoro-5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

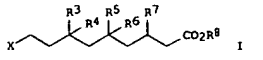
ACCESSION NUMBER: 2000:861451 CAPLUS
DOCUMENT NUMBER: 134:29136
TITLE: Novel nonanoic acid derivatives as alpha V integrin receptor antagonists
INVENTOR(S): Coleman, Paul J.; Duggan, Mark E.; Halczenko, Wasyl; Hartman, George D.; Hutchinson, John H.; Meissner, Robert S.; Patane, Michael A.; Perkins, James J.; Wang, Jiabing; Breslin, Michael J.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: PCT Int. Appl., 166 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000072801	A2	20001207	WO 2000-US14901	20000530
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2373937	AA	20001207	CA 2000-2373937	20000530
BR 2000011108	A	20020319	BR 2000-11108	20000530
EP 1187592	A2	20020320	EP 2000-942652	20000530
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200103431	T2	20020621	TR 2001-200103431	20000530
AU 749351	B2	20020627	AU 2000-57246	20000530
EE 200100642	A	20030217	EE 2001-642	20000530
JP 2004500326	T2	20040108	JP 2000-620913	20000530
US 6410526	B1	20020625	US 2000-583522	20000531
ZA 2001009837	A	20040310	ZA 2001-9837	20011129
NO 2001005858	A	20020204	NO 2001-5858	20011130
HR 2001000895	A1	20030831	HR 2001-895	20011130
BG 106232	A	20020628	BG 2001-106232	20011218

PRIORITY APPLN. INFO.: US 1999-137101P P 19990602
US 2000-179216P P 20000131
WO 2000-US14901 W 20000530

OTHER SOURCE(S): MARPAT 134:29136
GI

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



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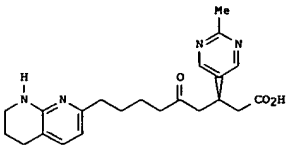


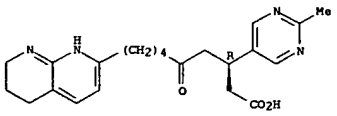
II

AB The invention discloses novel nonanoic acid derivs. I [X = substituted pyridine, pyrimidine, naphthyridine, etc; R3, R5 = H, OH, alkoxy; R4, R6 = H, alkyl; R3 and R4 or R5 and R6 taken together may form carbonyl oxygen; R7 = (un)substituted Ph, naphthyl, pyridyl, furyl, thienyl, etc.; R8 = H, alkyl] as αV integrin receptor antagonists along with methods for preparation Thus, compound II was prepared in eight steps from 6-oxo-heptanoic acid with chromatog. resolution of intermediate diketoester racemate. More particularly, the compds. of the present invention are antagonists of the integrin receptors αvβ3 and αvβ5, and are useful for inhibiting bone resorption, treating and preventing osteoporosis, and inhibiting vascular restenosis, diabetic retinopathy, macular degeneration, angiogenesis, atherosclerosis, inflammation, inflammatory arthritis, viral disease, cancer, and metastatic tumor growth.

IT **312261-73-7P 312261-74-8P 312262-00-3P 312262-01-4P 312262-03-6P 312262-04-7P 312262-06-9P 312262-07-0P 312262-09-2P 312262-10-5P 312262-12-7P 312262-13-8P 312262-15-0P 312262-16-1P 312262-21-8P 312262-22-9P 312262-24-1P 312262-25-2P 312262-35-4P 312262-36-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and biol. activity of nonanoic acid derivs. as αV integrin receptor antagonists)

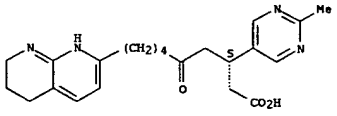
RN 312261-73-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



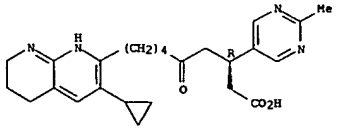
RN 312261-74-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



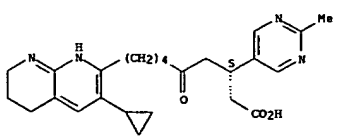
RN 312262-00-3 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312262-01-4 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

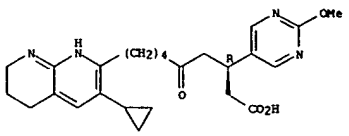
Absolute stereochemistry.



L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

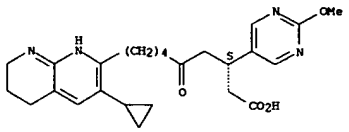
RN 312262-03-6 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



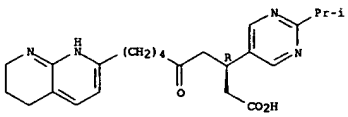
RN 312262-04-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



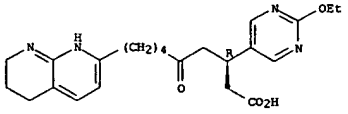
RN 312262-06-9 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-[2-(1-methylethyl)-5-pyrimidinyl]-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



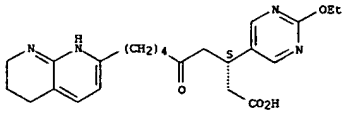
RN 312262-07-0 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-[2-(1-methylethyl)-5-pyrimidinyl]-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



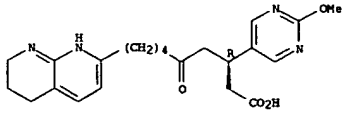
RN 312262-13-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, β-(2-ethoxy-5-pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



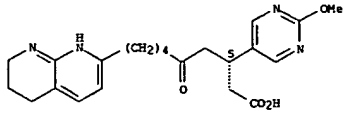
RN 312262-15-0 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312262-16-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

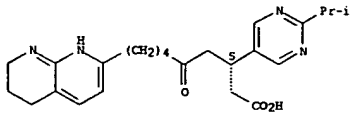
Absolute stereochemistry.



RN 312262-21-8 CAPLUS

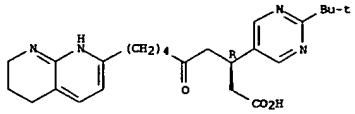
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

Absolute stereochemistry.



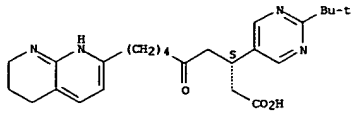
RN 312262-09-2 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, β-[2-(1,1-dimethylethyl)-5-pyrimidinyl]-1,5,6,7-tetrahydro-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312262-10-5 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, β-[2-(1,1-dimethylethyl)-5-pyrimidinyl]-1,5,6,7-tetrahydro-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

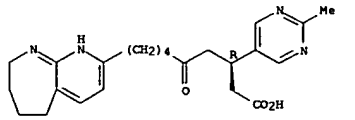


RN 312262-12-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, β-(2-ethoxy-5-pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

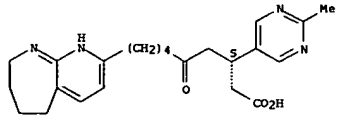
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



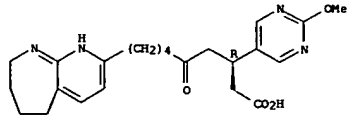
RN 312262-22-9 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312262-24-1 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

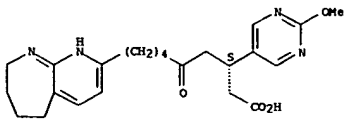
Absolute stereochemistry.



RN 312262-25-2 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

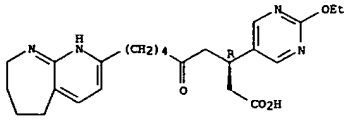
Absolute stereochemistry. Rotation (-).

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



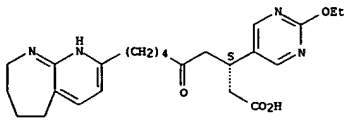
RN 312262-35-4 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, β-(2-ethoxy-5-pyrimidinyl)-5,6,7,8-tetrahydro-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312262-36-5 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, β-(2-ethoxy-5-pyrimidinyl)-5,6,7,8-tetrahydro-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 312261-69-1P 312261-70-4P 312261-71-5P
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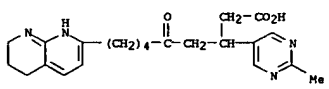
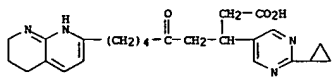
312262-61-6P 312262-62-7P 312262-63-8P

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 312261-72-6 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)

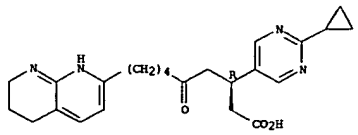


RN 312261-75-9 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, β-(2-cyclopropyl-5-pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo- (9CI) (CA INDEX NAME)



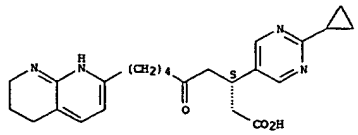
RN 312261-76-0 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, β-(2-cyclopropyl-5-pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312261-77-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, β-(2-cyclopropyl-5-pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

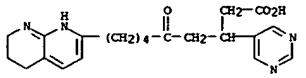
Absolute stereochemistry.



RN 312261-78-2 CAPLUS

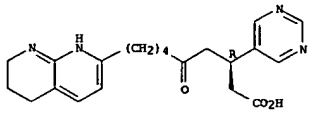
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
312262-64-9P 312262-65-0P 312262-66-1P
312262-67-2P 312262-68-3P 312262-69-4P
312262-70-7P 312262-71-8P 312262-72-9P
312262-76-3P 312262-77-4P 312262-78-5P
312262-79-6P 312262-80-9P 312262-81-0P
312262-85-4P 312262-86-5P 312262-87-6P
312262-88-7P 312262-89-8P 312263-62-0P
312263-63-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. and biol. activity of nonanoic acid derivs. as αV integrin receptor antagonists)

RN 312261-69-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-δ-oxo-β-5-pyrimidinyl- (9CI) (CA INDEX NAME)



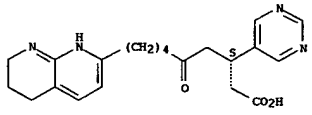
RN 312261-70-4 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-δ-oxo-β-5-pyrimidinyl-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

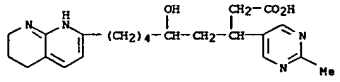


RN 312261-71-5 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-δ-oxo-β-5-pyrimidinyl-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

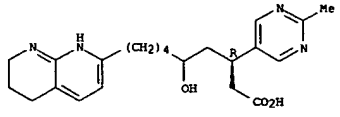


L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-δ-hydroxy-β-(2-methyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



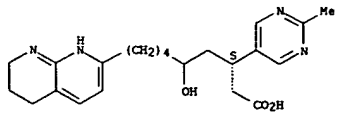
RN 312261-79-3 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-δ-hydroxy-β-(2-methyl-5-pyrimidinyl)-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

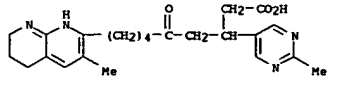


RN 312261-80-6 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-δ-hydroxy-β-(2-methyl-5-pyrimidinyl)-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

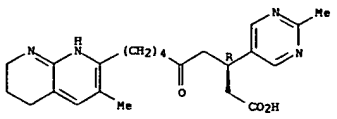


RN 312261-81-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-3-methyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



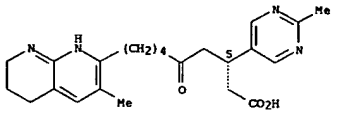
RN 312261-82-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-3-methyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

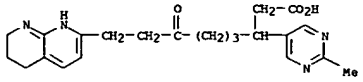


RN 312261-83-9 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-3-methyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

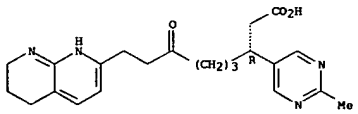


RN 312261-84-0 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-ζ-oxo- (9CI) (CA INDEX NAME)

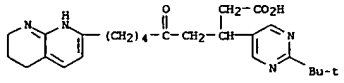


RN 312261-85-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-ζ-oxo-, (βR)- (9CI) (CA INDEX NAME)

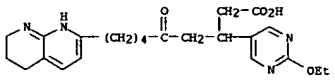
Absolute stereochemistry.



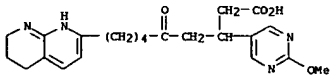
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



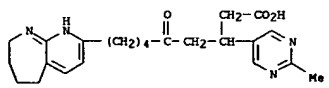
RN 312262-11-6 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, β-(2-ethoxy-5-pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo- (9CI) (CA INDEX NAME)



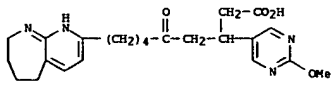
RN 312262-14-9 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



RN 312262-20-7 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



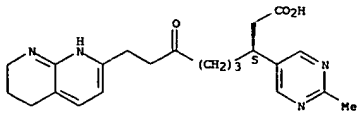
RN 312262-23-0 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, 5,6,7,8-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



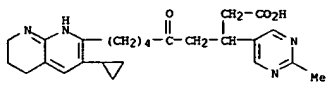
RN 312262-29-6 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-[6-[6-(methylamino)-2-pyridinyl]-2-

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 312261-86-2 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-ζ-oxo-, (βS)- (9CI) (CA INDEX NAME)

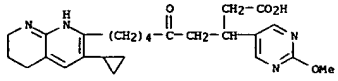
Absolute stereochemistry.



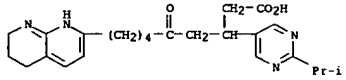
RN 312261-99-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



RN 312262-02-5 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)

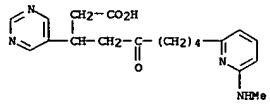


RN 312262-05-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-[2-(1-methylethyl)-5-pyrimidinyl]-δ-oxo- (9CI) (CA INDEX NAME)



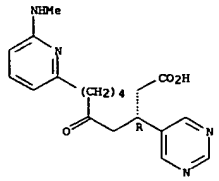
RN 312262-08-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, β-[2-(1,1-dimethylethyl)-5-pyrimidinyl]-1,5,6,7-tetrahydro-δ-oxo- (9CI) (CA INDEX NAME)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
oxohexyl]- (9CI) (CA INDEX NAME)



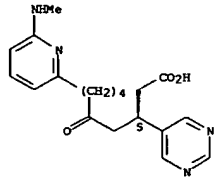
RN 312262-30-9 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-[6-[6-(methylamino)-2-pyridinyl]-2-oxohexyl]-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



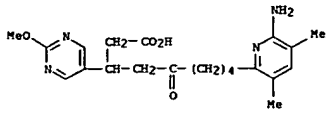
RN 312262-31-0 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-[6-[6-(methylamino)-2-pyridinyl]-2-oxohexyl]-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

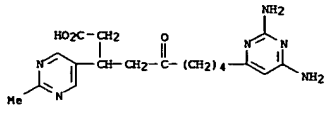


RN 312262-32-1 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-[6-(6-amino-3,5-dimethyl-2-pyridinyl)-2-oxohexyl]-2-methoxy- (9CI) (CA INDEX NAME)

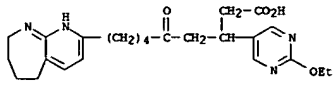
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



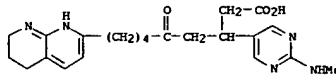
RN 312262-33-2 CAPLUS
CN 4-Pyrimidinenonanoic acid, 2,6-diamino-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



RN 312262-34-3 CAPLUS
CN 1H-Pyrido[2,3-b]azepine-2-nonanoic acid, β-(2-ethoxy-5-pyrimidinyl)-5,6,7,8-tetrahydro-δ-oxo- (9CI) (CA INDEX NAME)

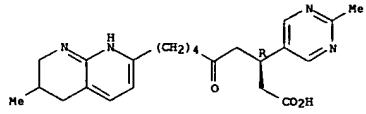


RN 312262-46-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-[2-(methylamino)-5-pyrimidinyl]-δ-oxo- (9CI) (CA INDEX NAME)



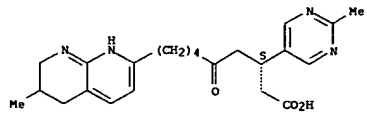
RN 312262-47-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-[2-(methylamino)-5-pyrimidinyl]-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

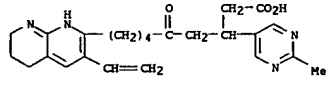


RN 312262-54-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-6-methyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

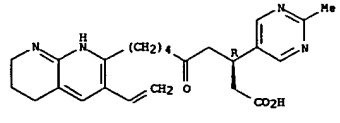


RN 312262-61-6 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-ethenyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



RN 312262-62-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-ethenyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

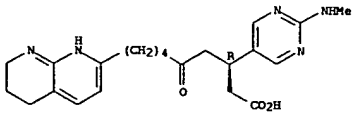
Absolute stereochemistry.



RN 312262-63-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-ethenyl-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

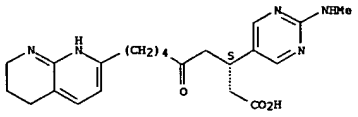
Absolute stereochemistry.

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.

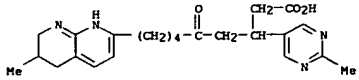


RN 312262-48-9 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-[2-(methylamino)-5-pyrimidinyl]-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



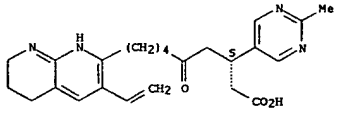
RN 312262-52-5 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-6-methyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



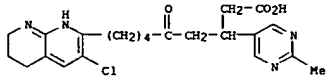
RN 312262-53-6 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-6-methyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

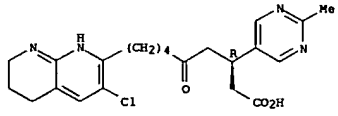


RN 312262-64-9 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-chloro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



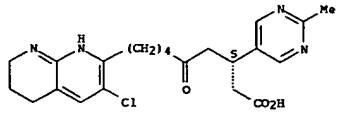
RN 312262-65-0 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-chloro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



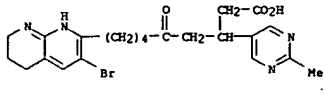
RN 312262-66-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-chloro-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



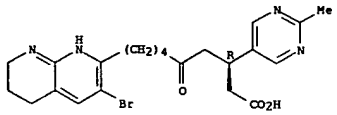
RN 312262-67-2 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-bromo-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



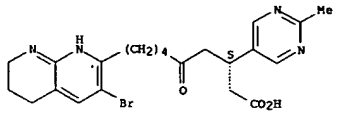
RN 312262-68-3 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-bromo-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

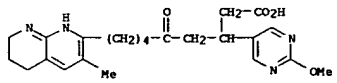


RN 312262-69-4 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-bromo-1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



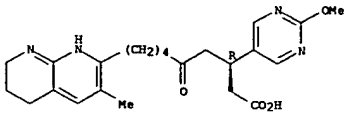
RN 312262-70-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-3-methyl-δ-oxo- (9CI) (CA INDEX NAME)



RN 312262-71-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-

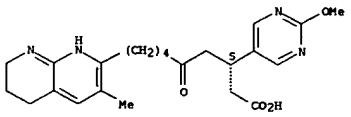
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
pyrimidinyl)-3-methyl-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

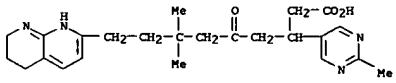


RN 312262-72-9 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-3-methyl-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



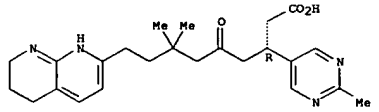
RN 312262-76-3 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-ζ,ζ-dimethyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo- (9CI) (CA INDEX NAME)



RN 312262-77-4 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-ζ,ζ-dimethyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

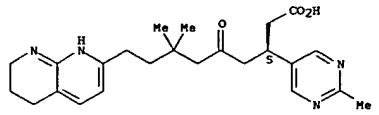
Absolute stereochemistry.

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

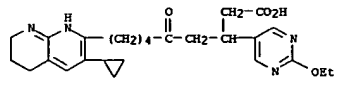


RN 312262-78-5 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-ζ,ζ-dimethyl-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

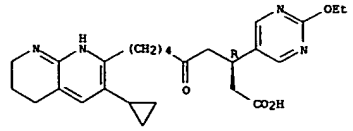


RN 312262-79-6 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-β-(2-ethoxy-5-pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo- (9CI) (CA INDEX NAME)



RN 312262-80-9 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-β-(2-ethoxy-5-pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

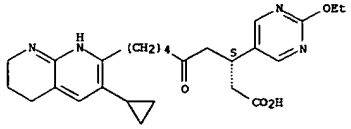
Absolute stereochemistry.



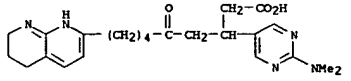
RN 312262-81-0 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-β-(2-ethoxy-5-

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
pyrimidinyl)-1,5,6,7-tetrahydro-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

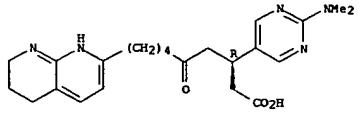


RN 312262-85-4 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, β-[2-(dimethylamino)-5-pyrimidinyl]-1,5,6,7-tetrahydro-δ-oxo- (9CI) (CA INDEX NAME)



RN 312262-86-5 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, β-[2-(dimethylamino)-5-pyrimidinyl]-1,5,6,7-tetrahydro-δ-oxo-, (βR)- (9CI) (CA INDEX NAME)

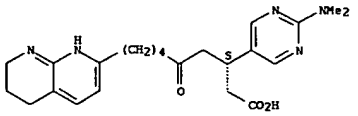
Absolute stereochemistry.



RN 312262-87-6 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, β-[2-(dimethylamino)-5-pyrimidinyl]-1,5,6,7-tetrahydro-δ-oxo-, (βS)- (9CI) (CA INDEX NAME)

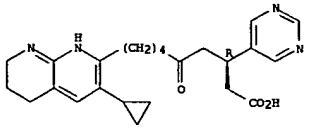
Absolute stereochemistry.

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



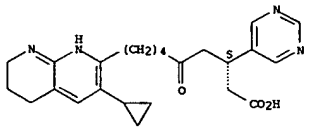
RN 312262-88-7 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-δ-oxo-β-5-pyrimidinyl-, (βR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312262-89-8 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 3-cyclopropyl-1,5,6,7-tetrahydro-δ-oxo-β-5-pyrimidinyl-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



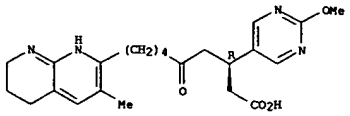
RN 312263-62-0 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-3-methyl-δ-oxo-, (βR)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 312262-71-8
CMF C23 H30 N4 O4

Absolute stereochemistry.

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



CM 2

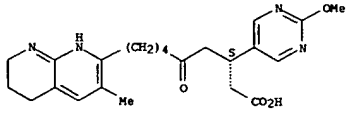
CRN 76-05-1
CMF C2 H F3 O2

RN 312263-63-1 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methoxy-5-pyrimidinyl)-3-methyl-δ-oxo-, (βS)-, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 312262-72-9
CMF C23 H30 N4 O4

Absolute stereochemistry.



CM 2

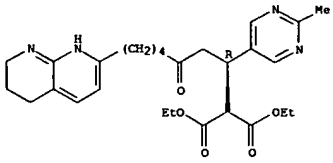
CRN 76-05-1
CMF C2 H F3 O2

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

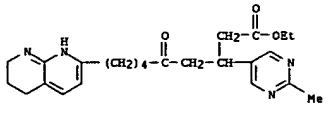
IT 312262-91-2P 312262-92-3P 312262-95-6P
312262-96-7P 312262-97-8P 312263-01-7P
312263-02-8P 312263-09-5P 312263-10-8P
312263-27-7P 312263-28-8P 312263-29-9P
312263-30-2P 312263-31-3P 312263-33-5P
312263-34-6P 312263-35-7P 312263-42-6P
312263-43-7P 312263-52-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and biol. activity of nonanoic acid derivs. as αV integrin receptor antagonists)

RN 312262-91-2 CAPLUS
CN Propanedioic acid, [(1R)-1-(2-methyl-5-pyrimidinyl)-3-oxo-7-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

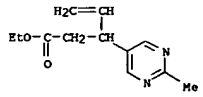


RN 312262-92-3 CAPLUS
CN 1,8-Naphthyridine-2-nonanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, ethyl ester (9CI) (CA INDEX NAME)

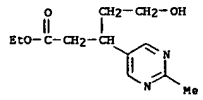


RN 312262-95-6 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-ethenyl-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)

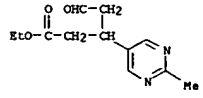
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 312262-96-7 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-(2-hydroxyethyl)-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)

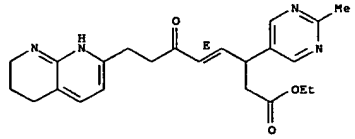


RN 312262-97-8 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methyl-β-(2-oxoethyl)-, ethyl ester (9CI) (CA INDEX NAME)



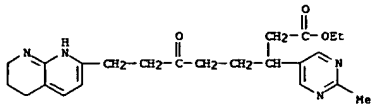
RN 312263-01-7 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methyl-β-[(1E)-3-oxo-5-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)-1-pentenyl]-, ethyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



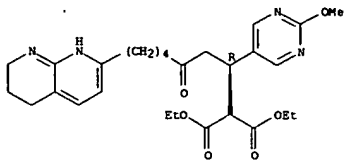
RN 312263-02-8 CAPLUS
CN 1,8-Naphthyridine-2-octanoic acid, 1,5,6,7-tetrahydro-β-(2-methyl-5-pyrimidinyl)-ε-oxo-, ethyl ester (9CI) (CA INDEX NAME)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



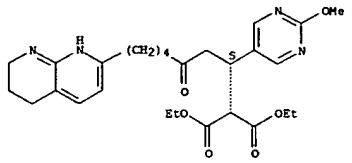
RN 312263-09-5 CAPLUS
CN Propanedioic acid, [(1R)-1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



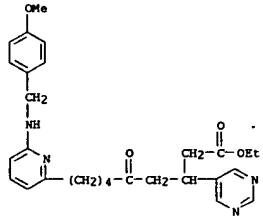
RN 312263-10-8 CAPLUS
CN Propanedioic acid, [(1S)-1-(2-methoxy-5-pyrimidinyl)-3-oxo-7-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

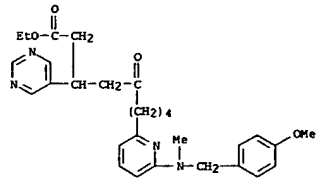


RN 312263-27-7 CAPLUS
CN Propanedioic acid, [(1S)-7-[6-[[(4-methoxyphenyl)methyl]amino]-2-pyridinyl]-3-oxo-1-(5-pyrimidinyl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

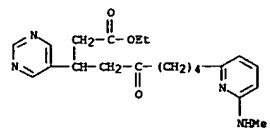
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 312263-30-2 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-[6-[6-[[(4-methoxyphenyl)methyl]methylamino]-2-pyridinyl]-2-oxohexyl]-, ethyl ester (9CI) (CA INDEX NAME)

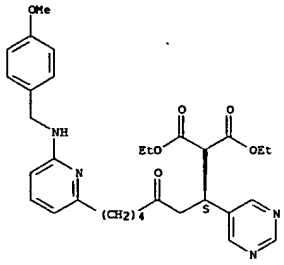


RN 312263-31-3 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-[6-[6-(methylamino)-2-pyridinyl]-2-oxohexyl]-, ethyl ester (9CI) (CA INDEX NAME)



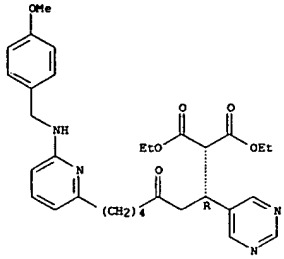
RN 312263-33-5 CAPLUS
CN Propanedioic acid, [1-(2-methyl-5-pyrimidinyl)-3-oxo-6-heptenyl]-, diethyl ester (9CI) (CA INDEX NAME)

L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Absolute stereochemistry.



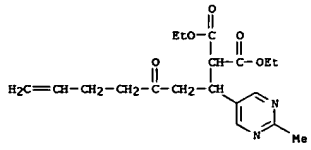
RN 312263-28-8 CAPLUS
CN Propanedioic acid, [(1R)-7-[6-[[(4-methoxyphenyl)methyl]amino]-2-pyridinyl]-3-oxo-1-(5-pyrimidinyl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

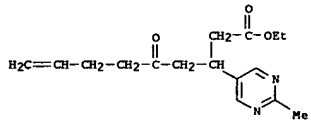


RN 312263-29-9 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-[6-[6-[[(4-methoxyphenyl)methyl]amino]-2-pyridinyl]-2-oxohexyl]-, ethyl ester (9CI) (CA INDEX NAME)

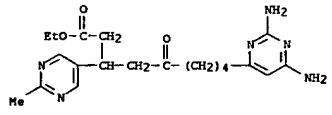
L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



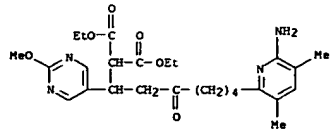
RN 312263-34-6 CAPLUS
CN 5-Pyrimidinepropanoic acid, 2-methyl-β-(2-oxo-5-hexenyl)-, ethyl ester (9CI) (CA INDEX NAME)



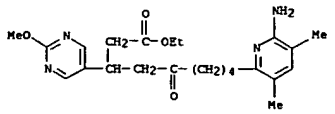
RN 312263-35-7 CAPLUS
CN 4-Pyrimidinenonanoic acid, 2,6-diamino-β-(2-methyl-5-pyrimidinyl)-δ-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 312263-42-6 CAPLUS
CN Propanedioic acid, [7-(6-amino-3,5-dimethyl-2-pyridinyl)-1-(2-methoxy-5-pyrimidinyl)-3-oxoheptyl]-, diethyl ester (9CI) (CA INDEX NAME)

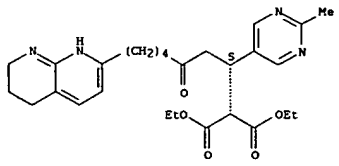


L7 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
RN 312263-43-7 CAPLUS
CN 5-Pyrimidinepropanoic acid, β-[6-(6-amino-3,5-dimethyl-2-pyridinyl)-2-oxohexyl]-2-methoxy-, ethyl ester (9CI) (CA INDEX NAME)

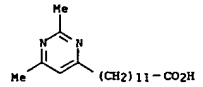


RN 312263-52-8 CAPLUS
CN Propanedioic acid, [(1S)-1-(2-methyl-5-pyrimidinyl)-3-oxo-7-(1,5,6,7-tetrahydro-1,8-naphthyridin-2-yl)heptyl]-, diethyl ester (9CI) (CA INDEX NAME)

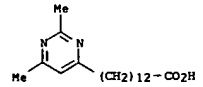
Absolute stereochemistry.



L7 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
C6H6 was added light petroleum (b. 60-80°) to turbidity, and the first yellow ppt. filtered off; addn. of more light petroleum pptd. 8.5 mg. 10-(2,6-dimethyl-4-pyrimidyl)-9-oxo-1-decanecarboxylic acid (VII), prisms, m. 96-7°. Similarly 2,6-dimethyl-4-pyrimidylmethyllithium heated with 10-bromo-1-decanecarboxylate, hydrolyzed, and treated with HCl gave 11-(2,6-dimethyl-4-pyrimidyl)-1-undecanecarboxylic acid (VIII), m. 94° (tuberculostatic activity of 1). 1-Bromodecanecarboxylic acid (22 g.) was refluxed with 19 cc. SOCl2 1 hr. and the excess of the reagent removed in vacuo; distn. gave a fraction (14.7 g.), b16 186°, which was added in 50 cc. dry Et2O during 15 min. at 0-5° to CH2N2 [from 30 g. MeN(NO)CONH2] in Et2O, the mixt. was kept at room temp. 1 hr., then evapd. in vacuo at 25°, the solid residue heated in 100 cc. dry EtOH to 55-60°, 6.8 g. dry Ag2O in 30 cc. dry EtOH added in portions, and the mixt. raised to b.p. and filtered; distn. gave 7 g. impure ethyl Br(CH2)11CO2Et (IX), isolated, hydrolyzed, and purified as described for VII to give platelets of 12-(2,6-dimethyl-4-pyrimidyl)-1-dodecanecarboxylic acid m. 96.5° [tuberculostatic activity 5 (loc. cit.)].
IT 857412-52-3, 4-Pyrimidinedodecanoic acid, 2,6-dimethyl-
857412-61-4, 4-Pyrimidinetridecanoic acid, 2,6-dimethyl-
(preparation of)
RN 857412-52-3 CAPLUS
CN 4-Pyrimidinedodecanoic acid, 2,6-dimethyl- (5CI) (CA INDEX NAME)



RN 857412-61-4 CAPLUS
CN 4-Pyrimidinetridecanoic acid, 2,6-dimethyl- (5CI) (CA INDEX NAME)



L7 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1954:32620 CAPLUS
DOCUMENT NUMBER: 48:32620
ORIGINAL REFERENCE NO.: 48:5865d-i,5866a
TITLE: Synthesis of potential antibacterial agents. II. A pyrimidine analog of chaulmoogric acid
AUTHOR(S): Heyes, T. D.; Roberts, John C.
SOURCE: Journal of the Chemical Society, Abstracts (1952) 4935-7
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 48:32620
AB cf. C.A. 45, 3332d. A general synthesis for ω-(2,6-dimethyl-4-pyrimidyl)alkane-1-carboxylic acids has been devised. Attempts to prepare ω-(2-pyrimidyl)- and ω-(5-pyrimidyl)alkane-1-carboxylic acids failed. Br(CH2)10CO2Et (I) (14.6 g.), 13 g. KCN, 100 cc. EtOH, and 20 cc. H2O refluxed 3 hrs., cooled, shaken with H2O, the insol. part dissolved in Et2O, the Et2O washed with H2O, dried (Na2SO4), and filtered; removal of Et2O and distillation in vacuo gave Et 10-cyano-1-decanecarboxylate (II), b11 196-8°. Dry HCl was passed into 5 g. II and 1 g. dry ice-cooled EtOH until 8.2 g. was absorbed, the mixture left at room temperature 14 hrs., 5 cc. Et2O added, the precipitated Et imidate-HCl filtered, dissolved in 15 cc. dry EtOH, dry 9% NH3-EtOH (50 cc.) added, the mixture shaken for 1 hr. then concentrated, the NH4Cl removed the filtrate evaporated, and the residue dissolved in O(CH2CH2OH)2, dry ether added, and the precipitate crystallized from C6H6, giving 2.0 g. 11-carbethoxyundecanamidine-HCl (III) as waxlike plates, m. 79°. III (1 g.) in 10 cc. EtOH added to 0.3 g. CH2Ac2 and 0.8 g. NaOEt in 15 cc. dry EtOH, the mixture kept 6 days at room temperature, diluted with 20 cc. H2O refluxed 1 hr., diluted with H2O, acidified, filtered, and the precipitate crystallized from aqueous EtOH gave 0.7 g. of 10-carbamoyl-1-decanecarboxylic acid (IV), prisms, m. 143°. Me H sebacate (20 g.) added to 60 g. SOCl2 and refluxed 4 hrs. yielded 9-carbomethoxynonanonyl chloride (V), b23 177°. To 7.14 g. PhLi in 150 cc. dry Et2O under N was added with stirring 10.4 g. 2,4,6-trimethylpyrimidine (VI) in 50 cc. dry Et2O, the mixture refluxed and stirred 15 min., treated with 18 g. V in 50 cc. dry Et2O, refluxed and stirred 3 hrs., let stand overnight under N, shaken with H2O, the Et2O layer extracted with 2N HCl, the acid exts. were made alkaline, extracted with Et2O, the exts. dried with MgSO4, filtered, the residue was refluxed 2.5 hrs. with 50 cc. 10% KOH in EtOH, diluted with H2O, extracted with Et2O, the aqueous layer was raised to pH 6.5, the emulsion extracted with Et2O, the extract dried, filtered, evaporated, the residue extracted with hot light petroleum (b. 100-20°). Cooling gave 0.05 g. crystals which were heated with C in MeOH and filtered; evaporation of the solvent and crystallization of the residue from light petroleum gave tan needles, to a solution of which in